ELSEVIER

31 March 1995

Chemical Physics Letters 235 (1995) 618–627

CHEMICAL PHYSICS LETTERS

Author index to volume 235

Achiba, Y., see N. Okabe 235 (1995) 564
Adamowicz, L., see G.L. Gutsev 235 (1995) 377
Ago, H., see K. Tanaka 235 (1995) 217
Ågren, H., see J. Guo 235 (1995) 152
Agulló-López, F., see M.A. Díaz-García 235 (1995) 535
Ahmad, I.K., see H.-B. Qian 235 (1995) 255
Al-Abbas, J., see B. Kozankiewicz 235 (1995) 456
Albrecht, U. and H. Bässler, Yield of geminate pair dissociation in an energetically random hopping system 235 (1995) 389
Alexandrov, A.L., see V.A. Schweigert 235 (1995) 221
Amos, R.D., see S.A.C. McDowell 235 (1995) 1
Andersson, P.O., T. Gillbro, A.E. Asato and R.S.H. Liu, Temperature and viscosity sensitive S_1 emission from a highly substituted triene 235 (1995) 76
Andrews, D.L., see A.A. Demidov 235 (1995) 327
Arrivo, S.M., T.P. Dougherty, W.T. Grubbs and E.J. Heilweil, Ultrafast infrared spectroscopy of vibrational CO-stretch up-pumping and relaxation dynamics of $W(CO)_6$ 235 (1995) 247
Asato, A.E., see P.O. Andersson 235 (1995) 76
Austin, S.J., P.W. Fowler, D.E. Manolopoulos and F. Zerbetto, The Stone–Wales map for C_{60} 235 (1995) 146

Bačić, Z., see T. Schröder 235 (1995) 316
Baeten, A., F. De Proft and P. Geerlings, Basicity of primary amines: a group properties based study of the importance of inductive (electronegativity and softness) and resonance effects 235 (1995) 17
Bak, K.L., see K. Ruud 235 (1995) 47
Balasubramanian, K., Geometry-dependent connectivity indices for the characterization of molecular structures 235 (1995) 580
Balasubramanian, K., Graph theoretical perception of molecular symmetry (Chemical Physics Letters 232 (1995) 415). Erratum 235 (1995) 394
Bässler, H., see U. Albrecht 235 (1995) 389
Becker, D., H. Yersin and A. von Zelewsky, Matrix deuteration effects and spin–lattice relaxation in the lowest triplet of the palladium(II) complex $Pd(2\text{-thpy})_2$ 235 (1995) 490
Becker, K.H., R. Kurtenbach, F. Schmidt and P. Wiesen, Temperature and pressure dependence of the $NCO + C_2H_2$ reaction 235 (1995) 230
Bedanov, V.M., see V.A. Schweigert 235 (1995) 221
Belle-Oudry, D.A., S. Satyapal, T. Mussillon and P.L. Houston, Detection of PO, Cl and P from the photodissociation of $POCl_3$ at 193 nm 235 (1995) 235

ELSEVIER

31 March 1995

Chemical Physics Letters 235 (1995) 618–627

CHEMICAL PHYSICS LETTERS

Author index to volume 235

Achiba, Y., see N. Okabe 235 (1995) 564
Adamowicz, L., see G.L. Gutsev 235 (1995) 377
Ago, H., see K. Tanaka 235 (1995) 217
Ågren, H., see J. Guo 235 (1995) 152
Agulló-López, F., see M.A. Díaz-García 235 (1995) 535
Ahmad, I.K., see H.-B. Qian 235 (1995) 255
Al-Abbas, J., see B. Kozankiewicz 235 (1995) 456
Albrecht, U. and H. Bässler, Yield of geminate pair dissociation in an energetically random hopping system 235 (1995) 389
Alexandrov, A.L., see V.A. Schweigert 235 (1995) 221
Amos, R.D., see S.A.C. McDowell 235 (1995) 1
Andersson, P.O., T. Gillbro, A.E. Asato and R.S.H. Liu, Temperature and viscosity sensitive S_1 emission from a highly substituted triene 235 (1995) 76
Andrews, D.L., see A.A. Demidov 235 (1995) 327
Arrivo, S.M., T.P. Dougherty, W.T. Grubbs and E.J. Heilweil, Ultrafast infrared spectroscopy of vibrational CO-stretch up-pumping and relaxation dynamics of $W(CO)_6$ 235 (1995) 247
Asato, A.E., see P.O. Andersson 235 (1995) 76
Austin, S.J., P.W. Fowler, D.E. Manolopoulos and F. Zerbetto, The Stone–Wales map for C_{60} 235 (1995) 146

Bačić, Z., see T. Schröder 235 (1995) 316
Baeten, A., F. De Proft and P. Geerlings, Basicity of primary amines: a group properties based study of the importance of inductive (electronegativity and softness) and resonance effects 235 (1995) 17
Bak, K.L., see K. Ruud 235 (1995) 47
Balasubramanian, K., Geometry-dependent connectivity indices for the characterization of molecular structures 235 (1995) 580
Balasubramanian, K., Graph theoretical perception of molecular symmetry (Chemical Physics Letters 232 (1995) 415). Erratum 235 (1995) 394
Bässler, H., see U. Albrecht 235 (1995) 389
Becker, D., H. Yersin and A. von Zelewsky, Matrix deuteration effects and spin–lattice relaxation in the lowest triplet of the palladium(II) complex $Pd(2\text{-thpy})_2$ 235 (1995) 490
Becker, K.H., R. Kurtenbach, F. Schmidt and P. Wiesen, Temperature and pressure dependence of the $NCO + C_2H_2$ reaction 235 (1995) 230
Bedanov, V.M., see V.A. Schweigert 235 (1995) 221
Belle-Oudry, D.A., S. Satyapal, T. Mussillon and P.L. Houston, Detection of PO, Cl and P from the photodissociation of $POCl_3$ at 193 nm 235 (1995) 235

Bergmann, K., see M. Rösslein 235 (1995) 242
Bieler, C.R., A. Sanov and H. Reisler, Inelastic scattering of NO($^2\Pi$) with atomic and molecular colliders. Rotational and fine-structure excitations 235 (1995) 175
Bigwood, R. and M. Gruebele, A simple matrix model of intramolecular vibrational redistribution and its implications 235 (1995) 604
Binder, H., see H. Heerklotz 235 (1995) 517
Binnemans, K. and C. Görller-Walrand, On the color of the trivalent lanthanide ions 235 (1995) 163
Blagoi, Y.P., see I.D. Reva 235 (1995) 617
Blume, A., see H. Heerklotz 235 (1995) 517
Boda, D., J. Liszi and I. Szalai, An extension of the NpT plus test particle method for the determination of the vapour–liquid equilibria of pure fluids 235 (1995) 140
Botschwina, P., see S. Schmatz 235 (1995) 5
Bouanah, N., see C. Fauquet 235 (1995) 528
Bourée, J.E., see C. Fauquet 235 (1995) 528
Bowman, J.M., see D. Wang 235 (1995) 277
Boyd, R.J., see L.A. Eriksson 235 (1995) 422
Bretón, J., see J. Hernández-Rojas 235 (1995) 160
Brillaud, P., see C. Fauquet 235 (1995) 528
Brugè, F., G. Cottone and S.L. Fornili, Solute–solute solvent-induced interaction: molecular dynamics simulation of a mixed model system in water 235 (1995) 402
Byers Brown, W., Photonucleation of water vapour in the presence of oxygen 235 (1995) 94
Bylaska, E., see P.R. Taylor 235 (1995) 558

Cai, R.-F., see J. Chen 235 (1995) 570
Campbell, M.L., R.E. McClean and J.S.S. Harter, Reaction kinetics of Mo(a^7S_3, a^5S_2, a^5D_J, a^5G_J) with O_2 235 (1995) 497
Canters, G.W., see J.W.A. Coremans 235 (1995) 202
Chakravorti, S., see A. Sarkar 235 (1995) 195
Chandra, A., Ion solvation dynamics in binary dipolar liquids: theoretical and simulation results for mixtures of Stockmayer liquids 235 (1995) 133
Chen, J., Q.-F. Shao, Z.-E. Huang, R.-F. Cai and S.-M. Chen, Solid-state magnetic resonance study of $KC_{60}(THF)_x$ 235 (1995) 570
Chen, S.-M., see J. Chen 235 (1995) 570
Chou, P.-T. and S. Studer Martinez, Reinvestigation of solvent catalyzed ground-state reverse proton transfer in 7-hydroxyquinoline 235 (1995) 463
Coremans, J.W.A., M. van Gastel, O.G. Poluektov, E.J.J. Groenen, T. den Blaauwen, G. van Pouderoyen, G.W. Canters, H. Nar, C. Hammann and A. Messerschmidt, An ENDOR and ESEEM study of the blue copper protein azurin 235 (1995) 202
Cottone, G., see F. Brugè 235 (1995) 402
Custodio, R., see N.H. Morgon 235 (1995) 436

Dannetun, P., see C. Fauquet 235 (1995) 528
Datta, B. and D. Mukherjee, Treatment of quasi-degeneracy in single-reference coupled-cluster theory. Separation of dynamical and nondynamical correlation effects 235 (1995) 31
Davies, P.B., see H.-B. Qian 235 (1995) 255
Demidov, A.A. and D.L. Andrews, Theory of polarized fluorescence and absorption in molecular complexes comprising two chromophores with non-parallel absorption and emission transition dipole moments 235 (1995) 327

Den Blaauwen, T., see J.W.A. Coremans 235 (1995) 202
Deng, F., see Y. Yue 235 (1995) 503
De Proft, F., see A. Baeten 235 (1995) 17
Dexheimer, S.L., W.A. Vareka, D. Mittleman, A. Zettl and C.V. Shank, Nonexponential relaxation in solid C_{60} via time-dependent singlet exciton annihilation 235 (1995) 552
Díaz-García, M.A., F. Agulló-López, W.E. Torruellas and G.I. Stegeman, Identification of two-photon states in phthalocyanines by third harmonic generation spectroscopy 235 (1995) 535
Dmitriev, Yu.Yu., see A.O. Mitrushenkov 235 (1995) 410
Dolejšek, Z., M. Fárník and Z. Herman, Dynamics of chemical reactions of doubly-charged ions. CF_2D^+ formation in collisions of CF_2^{2+} and D_2 235 (1995) 99
Domcke, W., see B. Wolfseder 235 (1995) 370
Dougherty, T.P., see S.M. Arrivo 235 (1995) 247
Du, Q., see G.A. Sefler 235 (1995) 347
Dubov, V. and H. Rabitz, Optimal control of molecular motion for δ-target probability density 235 (1995) 309
Duhamel, J., see A. Yekta 235 (1995) 119
Dunlop, J.R., see J.D. Tobiason 235 (1995) 268

El-Bayoumi, M.A., see R.L. Rucker 235 (1995) 471
Engel, Th., see H. Lanig 235 (1995) 58
Eriksson, L.A., J. Wang and R.J. Boyd, The interactions between alkali metals and C_2H_2. Density functional theory as an analytic tool 235 (1995) 422
Ermakova, E.A., see S.I. Kubarev 235 (1995) 591

Fang, J.-Y. and H. Guo, Four-dimensional quantum dynamics of the CH_3I/MgO photodissociation 235 (1995) 341
Fárník, M., see Z. Dolejšek 235 (1995) 99
Fauquet, C., P. Dannetun, C. Fredriksson, S. Stafström, J.E. Bourée, P. Brillaud, N. Bouanah and W.R. Salaneck, Electronic structure of trimethylamine alane in the solid state 235 (1995) 528
Fornili, S.L., see F. Brugè 235 (1995) 402
Fowler, P.W., see S.J. Austin 235 (1995) 146
Fredriksson, C., see C. Fauquet 235 (1995) 528
Freude, D., Enhanced resolution in the ^1H NMR spectra of zeolite H-ZSM-5 by heteronuclear dipolar-dephasing spin-echo MAS 235 (1995) 69

Gallogy, E.B., see K.-L. Han 235 (1995) 211
Gan, L., see D. Zhou 235 (1995) 548
Geerlings, P., see A. Baeten 235 (1995) 17
Gillbro, T., see P.O. Andersson 235 (1995) 76
Gomez Llorente, J.M., see J. Hernández-Rojas 235 (1995) 160
Görller-Walrand, C., see K. Binnemans 235 (1995) 163
Groenen, E.J.J., see J.W.A. Coremans 235 (1995) 202
Grubbs, W.T., see S.M. Arrivo 235 (1995) 247
Gruebele, M., see R. Bigwood 235 (1995) 604
Guo, H., see J.-Y. Fang 235 (1995) 341
Guo, J., P. Skytt, N. Wassdahl, J. Nordgren, Y. Luo, O. Vahtras and H. Ågren, Resonant and non-resonant X-ray scattering from C_{70} 235 (1995) 152

Gutsev, G.L. and L. Adamowicz, Relationship between the dipole moments and the electron affinities for some polar organic molecules 235 (1995) 377

Hada, M., see H. Takashima 235 (1995) 13
Hamilton, P.A., see H.-B. Qian 235 (1995) 255
Hammann, C., see J.W.A. Coremans 235 (1995) 202
Han, K.-L., H. Lin, E.B. Gallogy and W.M. Jackson, Total collision cross sections for C_{60} scattering by Ar, Kr and Xe 235 (1995) 211
Handy, N.C., see S.A.C. McDowell 235 (1995) 1
Handy, N.C., see A. Willetts 235 (1995) 286
Harris, C.B., see R.L. Rucker 235 (1995) 471
Harter, J.S.S., see M.L. Campbell 235 (1995) 497
Hashimoto, T., see K. Hirao 235 (1995) 430
Heerklotz, H., G. Lantzsch, H. Binder, G. Klose and A. Blume, Application of isothermal titration calorimetry for detecting lipid membrane solubilization 235 (1995) 517
Heilweil, E.J., see S.M. Arrivo 235 (1995) 247
Helgaker, T., see K. Ruud 235 (1995) 47
Herman, Z., see Z. Dolejšek 235 (1995) 99
Hernández-Rojas, J., J. Bretón and J.M. Gomez Llorente, On polarization effects in endohedral fullerene complexes 235 (1995) 160
Hirao, K., H. Nakano and T. Hashimoto, Multireference Møller–Plesset perturbation treatment for valence and Rydberg excited states of benzene 235 (1995) 430
Holovko, M.F., see Yu.V. Kalyuzhnyi 235 (1995) 355
Hosoito, N., see T. Sugimoto 235 (1995) 183
Houston, P.L., see D.A. Belle-Oudry 235 (1995) 235
Hu, H., see Y. Yue 235 (1995) 503
Huang, C., see D. Zhou 235 (1995) 548
Huang, Z.-E., see J. Chen 235 (1995) 570
Huber, J.R., see M. Rösslein 235 (1995) 242
Hummer, G., The numerical accuracy of truncated Ewald sums for periodic systems with long-range Coulomb interactions 235 (1995) 297
Hupp, J.T., see H. Lu 235 (1995) 521

Ishii, N. and T. Shimizu, Density functional theory calculations of isotropic hyperfine coupling constants of atoms and monohydrides 235 (1995) 614
Ivanov, A.Yu., see I.D. Reva 235 (1995) 617
Iwaizumi, M., see N. Okabe 235 (1995) 564

Jackson, W.M., see K.-L. Han 235 (1995) 211
Jiang, Y., see J. Liu 235 (1995) 576
Jordan, K.D., see D.E. Love 235 (1995) 479
Jørgensen, P., see K. Ruud 235 (1995) 47

Käb, G., see H. Lanig 235 (1995) 58
Kades, E., see M. Rösslein 235 (1995) 242
Kajiwara, A., see T. Kawakami 235 (1995) 414
Kalyuzhnyi, Yu.V., G. Stell and M.F. Holovko, Analytical solution of the multidensity OZ equation for polymerizing fluid 235 (1995) 355

Kamachi, M., see T. Kawakami 235 (1995) 414
Kaupp, M., V.G. Malkin, O.L. Malkina and D.R. Salahub, Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory 235 (1995) 382
Kawai, A., T. Okutsu and K. Obi, Anisotropic S_1–T_1 intersystem crossing of 1-chloromethylnaphthalene 235 (1995) 450
Kawai, R., see P.R. Taylor 235 (1995) 558
Kawakami, T., S. Yamanaka, W. Mori, K. Yamaguchi, A. Kajiwara and M. Kamachi, No-overlap and orientation principle for ferromagnetic interactions between nitroxide groups 235 (1995) 414
Kawata, S., see N. Okabe 235 (1995) 564
Kendrick, B. and R.T Pack, Recombination resonances in thermal $H + O_2$ scattering 235 (1995) 291
Kikuchi, K., see N. Okabe 235 (1995) 564
Kinugawa, T., Semi-classical Monte Carlo path integration without root searches 235 (1995) 395
Kitazawa, K., see K. Tanaka 235 (1995) 217
Klose, G., see H. Heerklotz 235 (1995) 517
König, G., see A. Lehmann 235 (1995) 65
Kothe, G., see E. van Faassen 235 (1995) 83
Kozankiewicz, B., J. Al-Abbas and J. Prochorow, Migration of electronic excitation energy in the charge-transfer crystal of pyromellitic dianhydride–phenanthrene 235 (1995) 456
Kubarev, S.I., I.S. Kubareva and E.A. Ermakova, The calculation of magnetic effects and RYDMR spectra for intermediate short-lived complexes of paramagnetic species 235 (1995) 591
Kubareva, I.S., see S.I. Kubarev 235 (1995) 591
Kuppermann, A., see Y.-S.M. Wu 235 (1995) 105
Kurtenbach, R., see K.H. Becker 235 (1995) 230
Kwok, W.M. and D.L. Phillips, Solvation effects and short-time photodissociation dynamics of CH_2I_2 in solution from resonance Raman spectroscopy 235 (1995) 260

Lanig, H., Th. Engel, G. Käb and F.W. Schneider, Fluorescence quenching by electron transfer in quinolinium betaines. Semiempirical and experimental studies 235 (1995) 58
Lantzsch, G., see H. Heerklotz 235 (1995) 517
Laukenmann, K., see E. van Faassen 235 (1995) 83
Leahy, D.J., see D.L. Osborn 235 (1995) 484
Lehmann, A., G. König and K.H. Rieder, He-diffraction study of defect correlated water adsorption on the CaF_2 (111) surface 235 (1995) 65
Levine, Y.K., see E. van Faassen 235 (1995) 83
Li, G.-Y., X.-C. Xu, Y. Liu and X.-W. Wu, Improvement of signal-to-noise ratio in remote NQR spectroscopy by high-speed sampling 235 (1995) 508
Li, J., see K. Tanaka 235 (1995) 217
Li, Y.S., see S. Veliah 235 (1995) 53
Lin, H., see K.-L. Han 235 (1995) 211
Liszi, J., see D. Boda 235 (1995) 140
Liu, J. and Y. Jiang, Degeneracy of C_{60} molecular graph 235 (1995) 576
Liu, R.S.H., see P.O. Andersson 235 (1995) 76
Liu, Y., see G.-Y. Li 235 (1995) 508
Liu, Z., see D. Zhou 235 (1995) 548
Love, D.E. and K.D. Jordan, Electron impact excitation of the singlet and triplet B_{1u} $\pi \rightarrow \pi^*$ states of ethylene near threshold 235 (1995) 479

Lu, H., V. Petrov and J.T. Hupp, Intervalence excitation of the Creutz–Taube ion. Resonance Raman and time-dependent scattering studies of Franck–Condon effects 235 (1995) 521
Lü, X., see X. Xu 235 (1995) 541
Luo, C., see D. Zhou 235 (1995) 548
Luo, Y., see J. Guo 235 (1995) 152

Mac, M., J. Najbar and J. Wirz, Fluorescence quenching of derivatives of anthracene by organic electron donors and acceptors in acetonitrile. Electron and proton transfer mechanism 235 (1995) 187
Mak, C.H., see Y. Wang 235 (1995) 37
Malkin, V.G., see M. Kaupp 235 (1995) 382
Malkina, O.L., see M. Kaupp 235 (1995) 382
Manolopoulos, D.E., see S.J. Austin 235 (1995) 146
Matsuura, H., see T. Sugimoto 235 (1995) 183
McClean, R.E., see M.L. Campbell 235 (1995) 497
McDowell, S.A.C., R.D. Amos and N.C. Handy, Molecular polarisabilities – a comparison of density functional theory with standard ab initio methods 235 (1995) 1
Messerschmidt, A., see J.W.A. Coremans 235 (1995) 202
Mezyk, S.P., Direct rate constant measurement of radical disulphide anion formation for cysteine and cysteamine in aqueous solution 235 (1995) 89
Millot, C., see J.-C. Soetens 235 (1995) 22
Miranda, P.B., see G.A. Sefler 235 (1995) 347
Mitrushenkov, A.O. and Yu.Yu. Dmitriev, Passing the several billion limit in FCI calculations on a mini-computer. A norm-consistent zero CI threshold estimate within the dynamic CI approach 235 (1995) 410
Mittal, J.P., see H. Mohan 235 (1995) 444
Mittleman, D., see S.L. Dexheimer 235 (1995) 552
Mohan, H. and J.P. Mittal, Formation of radical cations of chlorobenzene in aqueous solutions. A pulse radiolysis study 235 (1995) 444
Molin, Yu.N., see D.V. Stass 235 (1995) 511
Morgon, N.H., R. Custodio and J.M. Riveros, A theoretical study of isomeric $C_6H_4Br^-$ ions 235 (1995) 436
Mori, W., see T. Kawakami 235 (1995) 414
Morokov, Y.N., see V.A. Schweigert 235 (1995) 221
Mukherjee, D., see B. Datta 235 (1995) 31
Mussillon, T., see D.A. Belle-Oudry 235 (1995) 235

Najbar, J., see M. Mac 235 (1995) 187
Nakano, H., see K. Hirao 235 (1995) 430
Nakatsuji, H., see H. Takashima 235 (1995) 13
Nar, H., see J.W.A. Coremans 235 (1995) 202
Neumark, D.M., see D.L. Osborn 235 (1995) 484
Newsam, J.M., see S. Veliah 235 (1995) 53
Nordgren, J., see J. Guo 235 (1995) 152

Obi, K., see A. Kawai 235 (1995) 450
Ohba, Y., see N. Okabe 235 (1995) 564

Okabe, N., Y. Ohba, S. Suzuki, S. Kawata, K. Kikuchi, Y. Achiba and M. Iwaizumi, Fourier transform EPR studies of metallofullerene ($La@C_{82}$) in CS_2 solution 235 (1995) 564
Okutsu, T., see A. Kawai 235 (1995) 450
Olsen, J., see K. Ruud 235 (1995) 47
Osborn, D.L., D.J. Leahy, E.M. Ross and D.M. Neumark, Study of the predissociation of CH_3O $\tilde{A}(^2A_1)$ by fast beam photofragment translational spectroscopy 235 (1995) 484

Pack, R.T, see B. Kendrick 235 (1995) 291
Pandey, R., see S. Veliah 235 (1995) 53
Petrov, V., see H. Lu 235 (1995) 521
Phillips, D.L., see W.M. Kwok 235 (1995) 260
Plokhotnichenko, A.M., see I.D. Reva 235 (1995) 617
Poluektov, O.G., see J.W.A. Coremans 235 (1995) 202
Prochorow, J., see B. Kozankiewicz 235 (1995) 456
Pudlak, M., Effect of the molecular dynamics of exchanging groups on electron transport. Stochastic Liouville equation approach 235 (1995) 126

Qian, H.-B., P.B. Davies, I.K. Ahmad and P.A. Hamilton, Detection of the infrared laser spectrum of the PO_2 radical in the gas phase 235 (1995) 255

Rabitz, H., see V. Dubov 235 (1995) 309
Radchenko, E.D., see I.D. Reva 235 (1995) 617
Reisler, H., see C.R. Bieler 235 (1995) 175
Reva, I.D., A.M. Plokhotnichenko, S.G. Stepanian, A.Yu. Ivanov, E.D. Radchenko, G.G. Sheina and Y.P. Blagoi, The rotamerization of conformers of glycine isolated in inert gas matrices. An infrared spectroscopic study (Chem. Phys. Letters 232 (1995) 141). Erratum 235 (1995) 617
Rieder, K.H., see A. Lehmann 235 (1995) 65
Riveros, J.M., see N.H. Morgon 235 (1995) 436
Rohlfing, E.A., see J.D. Tobiason 235 (1995) 268
Ross, E.M., see D.L. Osborn 235 (1995) 484
Rösslein, M., E. Kades, K. Bergmann and J.R. Huber, Alignment detected photofragment yield spectroscopy demonstrated by photodissociation of *t*-butylnitrite in a supersonic jet 235 (1995) 242
Rucker, R.L., B.J. Schwartz, M.A. El-Bayoumi and C.B. Harris, Ultrafast dynamics of sterically hindered tetraphenylmethylbutadiene in liquids 235 (1995) 471
Ruud, K., T. Helgaker, J. Olsen, P. Jørgensen and K.L. Bak, A numerically stable orbital connection for the calculation of analytical Hessians using perturbation-dependent basis sets 235 (1995) 47

Salahub, D.R., see M. Kaupp 235 (1995) 382
Salaneck, W.R., see C. Fauquet 235 (1995) 528
Sanov, A., see C.R. Bieler 235 (1995) 175
Sarkar, A. and S. Chakravorti, A study on the spectroscopy and photophysics of N-phenyl pyrrole and N-phenyl pyrazole 235 (1995) 195
Satyapal, S., see D.A. Belle-Oudry 235 (1995) 235
Schinke, R., see T. Schröder 235 (1995) 316
Schmatz, S. and P. Botschwina, A theoretical investigation of four electronic states of C_6^- and the ground state of linear C_6 235 (1995) 5

Schmidt, F., see K.H. Becker 235 (1995) 230
Schneider, F.W., see H. Lanig 235 (1995) 58
Schröder, T., R. Schinke and Z. Bačić, Resonances in the UV photodissociation of the Ar · · · HCl van der Waals complex? An exact quantum 3D wave packet study 235 (1995) 316
Schwartz, B.J., see R.L. Rucker 235 (1995) 471
Schweigert, V.A., A.L. Alexandrov, Y.N. Morokov and V.M. Bedanov, Kinetics of carbon cluster isomerization: from tricyclic rings to fullerenes 235 (1995) 221
Sefler, G.A., Q. Du, P.B. Miranda and Y.R. Shen, Surface crystallization of liquid *n*-alkanes and alcohol monolayers studied by surface vibrational spectroscopy 235 (1995) 347
Selloni, A., see A. Vittadini 235 (1995) 334
Shank, C.V., see S.L. Dexheimer 235 (1995) 552
Shao, Q.-F., see J. Chen 235 (1995) 570
Sheina, G.G., see I.D. Reva 235 (1995) 617
Shen, Y.R., see G.A. Sefler 235 (1995) 347
Shimizu, T., see N. Ishii 235 (1995) 614
Simos, T.E., A new method for computing eigenvalues of the radial Schrödinger equation 235 (1995) 321
Skytt, P., see J. Guo 235 (1995) 152
Smeyers, Y.G. and M. Villa, On the dilemma of potential energy calculations with geometry optimization for spectroscopic purposes 235 (1995) 587
Snider, N., Effect of core nonsphericity on the entropy of simple liquids 235 (1995) 365
Soetens, J.-C. and C. Millot, Effect of distributing multipoles and polarizabilities on molecular dynamics simulations of water 235 (1995) 22
Stafström, S., see C. Fauquet 235 (1995) 528
Stass, D.V., B.M. Tadjikov and Yu.N. Molin, Manifestation of quantum coherence upon recombination of radical ion pairs in weak magnetic fields. Systems with equivalent nuclei 235 (1995) 511
Stegeman, G.I., see M.A. Díaz-García 235 (1995) 535
Stell, G., see Yu.V. Kalyuzhnyi 235 (1995) 355
Stepanian, S.G., see I.D. Reva 235 (1995) 617
Studer Martinez, S., see P.-T. Chou 235 (1995) 463
Sugimoto, T., M. Tsujii, H. Matsuura and N. Hosoito, Weak ferromagnetism below 12 K in a lithium tetrafluorotetracyanoquinodimethanide salt 235 (1995) 183
Sun, F., see D. Zhou 235 (1995) 548
Suzuki, S., see N. Okabe 235 (1995) 564
Szalai, I., see D. Boda 235 (1995) 140

Tadjikov, B.M., see D.V. Stass 235 (1995) 511
Takashima, H., M. Hada and H. Nakatsuji, Spin–orbit effect on the magnetic shielding constant using the ab initio UHF method: gallium and indium tetrahalides 235 (1995) 13
Tan, H., see D. Zhou 235 (1995) 548
Tanaka, K., H. Ago, K. Yoshizawa, T. Yamabe, J. Li and K. Kitazawa, An ESR analysis of $C_{60}S_{16}$ 235 (1995) 217
Taylor, P.R., E. Bylaska, J.H. Weare and R. Kawai, C_{20}: fullerene, bowl or ring? New results from coupled-cluster calculations 235 (1995) 558
Tobiason, J.D., J.R. Dunlop and E.A. Rohlfing, Dispersed fluorescence spectroscopy of jet-cooled DCO 235 (1995) 268

Toennies, J.P. and A.F. Vilesov, Novel low-energy vibrational states of foreign particles in fluid ^{4}He clusters 235 (1995) 596
Torruellas, W.E., see M.A. Díaz-García 235 (1995) 535
Tsujii, M., see T. Sugimoto 235 (1995) 183

Vahtras, O., see J. Guo 235 (1995) 152
Van Faassen, E., S. Weber, K. Laukenmann, G. Kothe and Y.K. Levine, Photoexcited EOSIN as an EPR spin probe 235 (1995) 83
Van Gastel, M., see J.W.A. Coremans 235 (1995) 202
Van Pouderoyen, G., see J.W.A. Coremans 235 (1995) 202
Varandas, A.J.C., $J = 0$ reactivity and cross-section in the $H + O_2$ reaction: is there a pronounced maximum as a function of energy? 235 (1995) 111
Vareka, W.A., see S.L. Dexheimer 235 (1995) 552
Veliah, S., R. Pandey, Y.S. Li, J.M. Newsam and B. Vessal, Density functional study of structural and electronic properties of cube-like MgO clusters 235 (1995) 53
Vessal, B., see S. Veliah 235 (1995) 53
Vilesov, A.F., see J.P. Toennies 235 (1995) 596
Villa, M., see Y.G. Smeyers 235 (1995) 587
Vittadini, A. and A. Selloni, Density functional study of H_2 desorption from monohydride and dihydride Si(100) surfaces 235 (1995) 334
Von Zelewsky, A., see D. Becker 235 (1995) 490

Wang, D. and J.M. Bowman, Complex L^2 calculations of bound states and resonances of HCO and DCO 235 (1995) 277
Wang, J., see L.A. Eriksson 235 (1995) 422
Wang, N.Q., see X. Xu 235 (1995) 541
Wang, Y. and C.H. Mak, Transferable tight-binding potential for hydrocarbons 235 (1995) 37
Wassdahl, N., see J. Guo 235 (1995) 152
Weare, J.H., see P.R. Taylor 235 (1995) 558
Weber, S., see E. van Faassen 235 (1995) 83
Wiesen, P., see K.H. Becker 235 (1995) 230
Willetts, A. and N.C. Handy, The anharmonic constants for a symmetric top 235 (1995) 286
Winnik, M.A., see A. Yekta 235 (1995) 119
Wirz, J., see M. Mac 235 (1995) 187
Wolfseder, B. and W. Domcke, Multi-mode vibronic coupling with dissipation. Application of the Monte Carlo wavefunction propagation method 235 (1995) 370
Wu, X.-W., see G.-Y. Li 235 (1995) 508
Wu, Y.-S.M. and A. Kuppermann, The importance of the geometric phase effect for the $H + D_2 \rightarrow HD + D$ reaction 235 (1995) 105
Wu, Z., see D. Zhou 235 (1995) 548

Xia, X., see D. Zhou 235 (1995) 548
Xia, Z., see D. Zhou 235 (1995) 548
Xu, X., X. Lü, N.Q. Wang and Q.E. Zhang, Charge-consistency modelling of CO/NiO(100) chemisorption system 235 (1995) 541
Xu, X.-C., see G.-Y. Li 235 (1995) 508

Yamabe, T., see K. Tanaka 235 (1995) 217
Yamaguchi, K., see T. Kawakami 235 (1995) 414
Yamanaka, S., see T. Kawakami 235 (1995) 414
Ye, C., see Y. Yue 235 (1995) 503
Yekta, A., J. Duhamel and M.A. Winnik, Dipole–dipole electronic energy transfer. Fluorescence decay functions for arbitrary distributions of donors and acceptors: systems with planar geometry 235 (1995) 119
Yersin, H., see D. Becker 235 (1995) 490
Yoshimori, A., Nonlinear quantum effects on electron transfer reactions 235 (1995) 303
Yoshizawa, K., see K. Tanaka 235 (1995) 217
Yue, Y., F. Deng, H. Hu and C. Ye, ^{23}Na NMR studies of doped nasicon systems 235 (1995) 503

Zerbetto, F., see S.J. Austin 235 (1995) 146
Zettl, A., see S.L. Dexheimer 235 (1995) 552
Zhang, Q.E., see X. Xu 235 (1995) 541
Zhang, S., see D. Zhou 235 (1995) 548
Zhao, X., see D. Zhou 235 (1995) 548
Zhou, D., L. Gan, C. Luo, H. Tan, C. Huang, Z. Liu, Z. Wu, X. Zhao, X. Xia, S. Zhang, F. Sun, Z. Xia and Y. Zou, Langmuir–Blodgett film and nonlinear optical property of C_{60}–glycine ester derivative 235 (1995) 548
Zou, Y., see D. Zhou 235 (1995) 548